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Faster water dissociation fluctuations on the surface of Cassiterite[1] NITIN KUMAR, Department of Physics, The Pennsylvania State University, PAUL KENT, Center for Nanophase Materials Sciences and Chemical Sciences Division, Oak Ridge National Laboratory, ANDREI BANDURA, St. Petersburg State University, DAVID COLE, DAVID WESOLOWSKI, Chemical Sciences Division, Oak Ridge National Laboratory, JAMES KUBICKI, Department of Geosciences, The Pennsylvania State University, JORGE SOFO, Department of Physics, The Pennsylvania State University — We investigated water dissociation dynamics on rutile (110) surface (titanium dioxide) and cassiterite (110) surface (tin dioxide) using molecular dynamics simulation. We find that dissociation events occur around five times more frequently on cassiterite compared to rutile. The water on cassiterite surface is found to be closer to the surface due to stronger hydrogen bond formation between water and the surface. The increase in the strength of hydrogen bond is confirmed by a red shift of frequency OH vibrations at the surface. We will provide evidence that the origin of the stronger hydrogen bond on the surface of cassiterite resides in higher covalency between water and the bridging oxygen atoms at the surface.

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